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Title: Software and Files Index

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Software and Files Index

The purpose of this document is to provide an index of the software and files used to generate the results and findings documented in Section 4 of the scoping study report on Radiation Signatures relevant to Thorium Fuel Cycles.

Authors and Data Owners

This data was created and compiled by (in alphabetical order):

Eric Cervi, Andrea Favalli, Vlad Henzl, Madeline Lockhart, David Mercer, and Jacob Stinnett from Safeguards Science and Technology Group (NEN-1) at Los Alamos National Laboratory.

This data is made openly available to the safeguards community for reference. Please contact Vlad Henzl (henzl@lanl.gov) regarding further use and publication of this data, for appropriate citations and any future updates to these files.

Software

GADRAS 18.8.1 – Simulation of gamma measurement, results in form of a spectrum.

Reference: GADRAS Version 18 User's Manual. Steven M. Horne, Gregory G. Thoreson, Lisa A. Theisen, Dean J. Mitchell, Lee T. Harding, and Sean E. O'Brien. SAND2019-14305

Note: For each simulation, a 1-D model was defined using parameters specified for a specific scenario as discussed in Section 4 of the “Assessment of Safeguards Technology R&D Needs for Thorium Fuel Cycles” (e.g. mass of ^{233}U , its chemical and physical form, level of ^{232}U impurities, detector type, length of measurement, etc.). Spectra were generated with the “Inject” tool using default parameters of detector response functions.

PeakEasy 4.98 – analysis of simulated or experimentally obtained gamma spectra

Reference: Rooney, B., Garner, S., Felsher, P., Karpus, P., (2018), PeakEasy 4.98 [Computer Program], Los Alamos National Laboratory, Release LA-CC-13-040, <https://PeakEasy.lanl.gov>.

DeCayculator: - calculation of activities of ^{233}U and ^{232}U decay chains products

Reference: P. Karpus. The DeCayculator, Beta Version 1.0., Los Alamos National Laboratory, LA-CC-11-82; ICRP, 1983. Radionuclide Transformations - Energy and Intensity of Emissions. ICRP Publication 38. Ann. ICRP 11-13.

Note: LANL-internal code to compute activities of ^{233}U and ^{232}U decay chain products over time, based on ICRP 38 nuclear data. This calculated activities over time for then served as input for to calculate dose rates over time.

Files

Reports documents:

- **DoseCalculations.xlsx:** Contains data used for activity and dose over time figures. Activity data generated with Decayculator, and dose rate information is from PeakEasy. See Appendix A.
- **Files and Software Index.docx:** this file
- **RefData.xlsx:** reference data for uranium and thorium, such as half-lives, specific power (for calorimetry), spontaneous fission rates, etc.. See Appendix B
- **ThoriumMeasurements.xlsx:** compilation of neutron rates (S, D, T) measured with AWCC and ENMC detector during assay of various ^{252}Cf , Pu and Th and items. See Appendix C

GADRAS files

- **Thorium.pcf:** a GADRAS-generated spectra file with four spectra inside, numbered 1-4 (note: file generically named “Thorium” as it was created for the Th-safeguards project, however it contains all relevant spectra, some only with ^{233}U). See Appendix D
 1. Uses the ThoriumBall.1dm model
 2. Uses the ThoriumBall.1dm model
 3. Uses the U233Ball.1dm model
 4. Uses the U233Ball.1dm model
- **ThoriumBall.1dm:** a GADRAS 1-D model file of a 1 kg thorium oxide item. See Appendix E
- **U233.1dm:** a GADRAS 1-D model file of a 10-gram U-233 metal item. See Appendix E
- **ThoriumBall.gam:** a GADRAS gamma file; contains the physics data generated by the associated 1-D mode. See Appendix F
- **U233Ball.gam:** a GADRAS gamma file; contains the physics data generated by the associated 1-D model. See Appendix F.

General Item Properties		Total U Mass (g)		²³⁵ U contamination (ppm)																						
		1.00																								
		10.0																								
Item properties by isotope:																										
Nuclide	[wt%]	Activity [k ⁻¹]	Activity [%]																							
²³⁵ U	0.001	2.24E-02	2.25																							
²³⁸ U	99.999	0.9699903	97.75																							
Raw Decayculator Results - ²³⁵ U decay																										
Nuclide	0.00274	0.02	0.1	0.25	0.5	0.75	1	1.5	2	2.5	3	4	5	6	7	8	9	10	12.5	15	17.5	20	25	30	50	100
²³⁵ U	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00
²³⁸ U	2.59E-07	1.89E-06	9.42E-06	2.36E-05	4.72E-05	7.08E-05	9.44E-05	0.000124	0.000168	0.000212	0.000256	0.000300	0.000344	0.000388	0.000432	0.000476	0.000520	0.000564	0.000608	0.000652	0.000696	0.000740	0.000784	0.000828	0.000872	0.000916
²³⁹ Pa	5.97E-09	2.89E-07	4.94E-06	1.27E-05	4.17E-05	6.53E-05	8.89E-05	0.000116	0.000143	0.000170	0.000197	0.000224	0.000251	0.000278	0.000305	0.000332	0.000359	0.000386	0.000413	0.000440	0.000467	0.000494	0.000521	0.000548	0.000575	0.000602
²³⁸ Th	1.36E-10	4.43E-08	2.65E-06	1.46E-05	3.80E-05	6.16E-05	8.52E-05	0.000108	0.000136	0.000164	0.000192	0.000220	0.000248	0.000276	0.000304	0.000332	0.000360	0.000388	0.000416	0.000444	0.000472	0.000500	0.000528	0.000556	0.000584	0.000612
²³⁴ Th	1.34E-10	2.64E-08	1.44E-06	3.90E-05	6.16E-05	8.52E-05	0.000108	0.000136	0.000164	0.000192	0.000220	0.000248	0.000276	0.000304	0.000332	0.000360	0.000388	0.000416	0.000444	0.000472	0.000500	0.000528	0.000556	0.000584	0.000612	0.000640
²³⁴ Pa	1.34E-10	4.42E-08	2.64E-06	1.46E-05	3.80E-05	6.16E-05	8.52E-05	0.000108	0.000136	0.000164	0.000192	0.000220	0.000248	0.000276	0.000304	0.000332	0.000360	0.000388	0.000416	0.000444	0.000472	0.000500	0.000528	0.000556	0.000584	0.000612
²³⁴ Th	1.18E-10	4.25E-08	2.64E-06	1.46E-05	3.80E-05	6.16E-05	8.52E-05	0.000108	0.000136	0.000164	0.000192	0.000220	0.000248	0.000276	0.000304	0.000332	0.000360	0.000388	0.000416	0.000444	0.000472	0.000500	0.000528	0.000556	0.000584	0.000612
²³⁴ Pa	1.15E-10	4.35E-08	2.64E-06	1.46E-05	3.80E-05	6.16E-05	8.52E-05	0.000108	0.000136	0.000164	0.000192	0.000220	0.000248	0.000276	0.000304	0.000332	0.000360	0.000388	0.000416	0.000444	0.000472	0.000500	0.000528	0.000556	0.000584	0.000612
²³⁴ Th	6.92E-12	9.38E-10	5.71E-08	3.17E-07	8.20E-07	1.33E-06	1.84E-06	2.66E-06	3.88E-06	4.90E-06	6.22E-06	7.66E-06	9.00E-06	1.05E-05	1.20E-05	1.41E-05	1.61E-05	1.82E-05	2.03E-05	2.23E-05	2.44E-05	2.65E-05	2.86E-05	3.07E-05	3.28E-05	3.49E-05
²³⁴ Pa	2.51E-11	4.03E-09	2.51E-08	1.45E-07	3.79E-07	6.1																				

Nuclide	Gamma Dose [Rem/hr@1m/Cl] ["]	Specific Activity [Ci/g]	Primary Decay Mode	Atomic weight	Alpha energy [keV] ["]	Beta endpoint E [keV] ["]
²³³ U	2.60E-04	0.0097	α	233	4908	-
²²⁹ Th	3.23E-02	0.2126	α	229	5167	-
²²⁶ Ra	3.18E-02	3.92E+04	β ⁻	225	-	357
²²⁶ Ac	8.20E-03	5.80E+04	α	225	5935.1	-
²²¹ Fr	4.41E-02		α	221	6458.1	-
²¹⁷ At	1.60E-04		99.99% α	217	7201.9	-
²¹³ Bi	8.72E-02	1.93E+07		213	5982	-
²¹³ Po	1.94E-05	1.26E+16	α	213	8537	-
²⁰⁸ Tl	1.29E+00	4.09E+08	β ⁻	209	-	3980
²⁰⁸ Pb				209	-	-
²³² U	0.00024	2.24E+01	α	232	5413.55	-
²²⁸ Th	0.00164	8.25E+02	α	228	5520.12	-
²²⁴ Ra	0.00739	1.59E+05	α	224	5788.87	-
²²⁰ Rn	0.00043	9.22E+08	α	220	6404.67	-
²¹⁶ Po	8.97E-06		α	216	6906.5	-
²¹² Pb	0.273393		β ⁻	212	-	573.7
²¹² Bi	0.0615	1.46E+07	64.06% beta, 35.94% α	212	6207.14	2254
²¹² Po		1.80E+17	α	212	8954.13	-
²⁰⁸ Tl	1.63	2.92E+08	β ⁻	208	-	5000.9

[**] <http://nucldata.nuclear.lu.se/toi/abouttoi.htm>

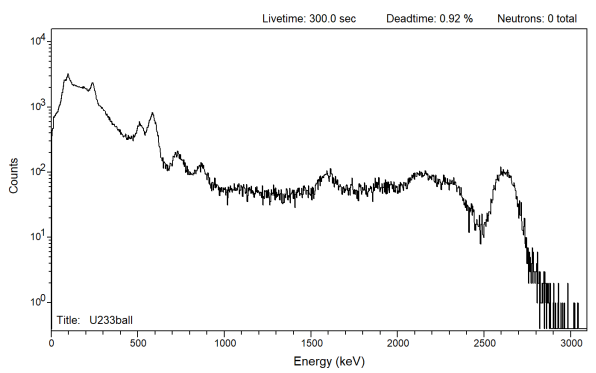
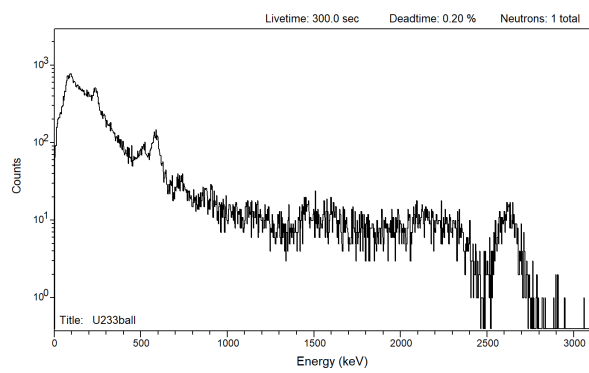
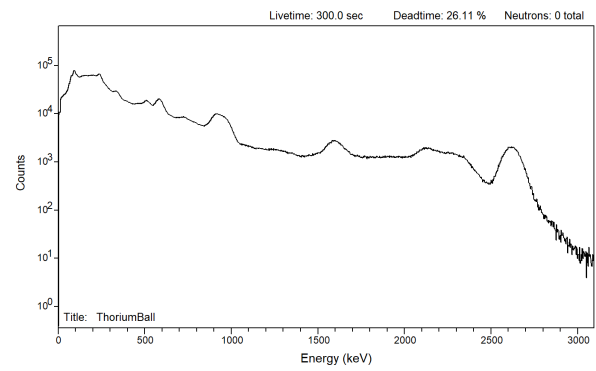
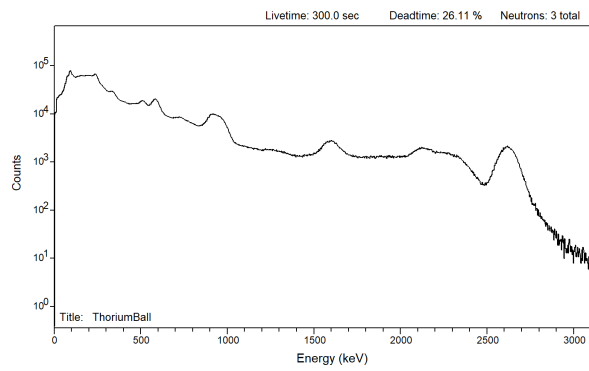
Appendix B: RefData.xlsx

Nuclide	Half life	Primary Decay Mode	Spontaneous Fission Rate - SF [s ⁻¹ .kg ⁻¹]	Fission Cross Section - σ [b]; fission spectrum avg	SF Neutron Multiplicity - ν_{SF} [1]	Fission Spectrum Neutron Multiplicity - ν_{FS} [1]	Critical Mass - M_c [kg]	Decay Heat - Q [W/kg]	Specific Activity [Ci/kg]
²³² Th	1.405 x 10 ¹⁰ y	Alpha 4.083 MeV	<5 x 10 ⁻⁶	0.0785	-	2.16	None	2.654 x 10 ⁻⁶	1.097 x 10 ⁻⁴
²³¹ Pa	32760 y	Alpha 5.149 MeV	<5	0.834	-	2.457	>188	1.442	47.23
²³² U	68.9 y	Alpha 5.414 MeV	2 x 10 ⁻³	2.013	2	3.296	>5	717.6	22,360
²³³ U	159200 y	Alpha 4.909 MeV	-	1.946	-	2.649	16	0.2804	9.636
²³⁴ U	245500 y	Alpha 4.859 MeV	3.9	1.223	1.8	2.578	>41	0.1792	6.222
²³⁵ U	7.038 x 10 ⁸ y	Alpha 4.679 MeV	5.6 x 10 ⁻³	1.235	2	2.6055	48	5.994 x 10 ⁻⁵	2.161 x 10 ⁻³
²³⁶ U	2.342 x 10 ⁷ y	Alpha 4.572 MeV	2.3	0.594	1.8	2.526	>167	1.753 x 10 ⁻³	0.06467
²³⁸ U	4.468 x 10 ⁹ y	Alpha 4.270 MeV	5.51	0.308	1.97 ± 0.07	2.601	None	8.508 x 10 ⁻⁶	3.361 x 10 ⁻⁴
²³⁷ Np	2.144 x 10 ⁶ y	Alpha 4.959 MeV	< 0.05	1.335	2	2.889	75-105	0.02068	0.7034
²³⁸ Pu	87.7 y	Alpha 5.593 MeV	1.204 x 10 ⁶	1.994	2.28 ± 0.10	3.148	9	5.678 x 10 ⁵	17,120
²³⁹ Pu	24110 y	Alpha 5.245 MeV	10.1	1.8	2.9	3.1231	10.5	1.929	62.03
²⁴⁰ Pu	65640 y	Alpha 5.256 MeV	478,000	1.357	2.189 ± 0.026	3.061	40	7.07	227
²⁴¹ Pu	14.35 y	Beta 0.021 MeV	<0.8	1.648	-	3.142	12	129.4	1.033 x 10 ⁵
²⁴² Pu	373300 y	Alpha 4.984 MeV	805,000	1.127	2.28 ± 0.13	3.07	95, range 75-100	0.1169	3.956
²⁴¹ Am	432.2 y	Alpha 5.638 MeV	500	1.378	2	3.457	83.5	114.7	3,431
²⁵¹ Cf	898 y	Alpha 6.176 MeV	-	2.43	-	4.56	1.94	58.05	1,586

Appendix C: ThoriumMeasurements.xlsx

ACTIVE Measurements														
AWCC		No Cd liner, No Ni	8/21/2019	Note: ²⁵² Cf in bottom plug, ²³² Th on 7 cm stand in cavity										
Items	Measurement time	²³² Th mass [g]	Singles	σ	Doubles	σ	Triples	σ	Δ Singles	σ	Δ Doubles	σ	Δ Triples	σ
bkg	60 x 20s = 20 min	0	21.62	0.34	0.345	0.025	0.027	0.006	-	-	-	-	-	-
FTC-CF-1992	60 x 20s = 20 min	0	47466.8	7.2	4256.3	10.6	232.0	17.9	-	-	-	-	-	-
FTC-CF-1992, TH-5D	90 x 20s = 30 min	31.5	47351.1	5.2	4231.9	10.2	232.8	14.3	-115.75	8.86	-24.37	14.75	0.84	22.92
FTC-CF-1992, TH-5D, TH-6D	90 x 20s = 30 min	59.5	47406.1	5.2	4256.7	10.0	208.2	12.7	-60.75	8.86	0.43	14.60	-23.79	21.96
FTC-CF-1992, TH-5D, TH-6D, TH-9D, TH-10D	90 x 20s = 30 min	89.2	47396.8	6.6	4245.9	10.3	235.7	15.5	-70.01	9.76	-10.36	14.80	3.68	23.69
AWCC		With Cd liner, No Ni	8/22/2019	Note: ²⁵² Cf in bottom plug, ²³² Th on 7 cm stand in cavity										
Items	Measurement time	²³² Th mass [g]	Singles	σ	Doubles	σ	Triples	σ	Δ Singles	σ	Δ Doubles	σ	Δ Triples	σ
FTC-CF-1992	120 x 20s = 40 min	0	34535.3	4.4	3309.4	6.2	185.5	7.6	-	-	-	-	-	-
FTC-CF-1992, TH-5D, TH-6D, TH-9D, TH-10D	120 x 20s = 40 min	89.2	34412.4	4.6	3291.0	6.8	181.5	8.3	-122.92	6.36	-18.36	9.17	-4	11.22
ENMC			8/22/2019	Note: ²⁵² Cf on rod, ²³² Th on 7 cm stand in cavity										
Items	Measurement time	²³² Th mass [g]	Singles	σ	Doubles	σ	Triples	σ	Δ Singles	σ	Δ Doubles	σ	Δ Triples	σ
FTC-CF-1992	120 x 20s = 40 min	0	229281.5	16.7	141382.3	49.4	50580	137	-	-	-	-	-	-
FTC-CF-1992, TH-5D, TH-6D, TH-9D, TH-10D	120 x 20s = 40 min	89.2	229235.2	17.6	141350.0	56.0	50593	148	-46.27	24.27	-32.29	74.66	12.605	201.31
AWCC		With Cd liner, with Ni	7/30/2019	Note: AmLi in top plug, ²³² Th on stand in cavity										
Items	Measurement time	²³² Th mass [g]	Singles	σ	Doubles	σ	Triples	σ	Δ Singles	σ	Δ Doubles	σ	Δ Triples	σ
N-471	106 x 30s = 53 min	0	2341.53	0.87	1.15	0.32	0.24	0.10	-	-	-	-	-	-
N-471, TH-10D	90 x 30s = 45 min	15	2346.06	0.90	0.73	0.34	0.38	0.11	4.53	1.25	-0.42	0.47	0.141	0.15
PASSIVE Measurements														
ENMC		6/27/2019												
Items	Measurement time	²³² Th mass [g]	Singles	σ	Doubles	σ	Triples	σ						
Ni-TH3KG		3000	1.68	0.58	1.67	0.89	3.3	2.2						
TH-10D		15	0.29	0.48	0.53	0.18	0.68	0.33						

Appendix D: Thorium.pcf, which also contains U233 output.



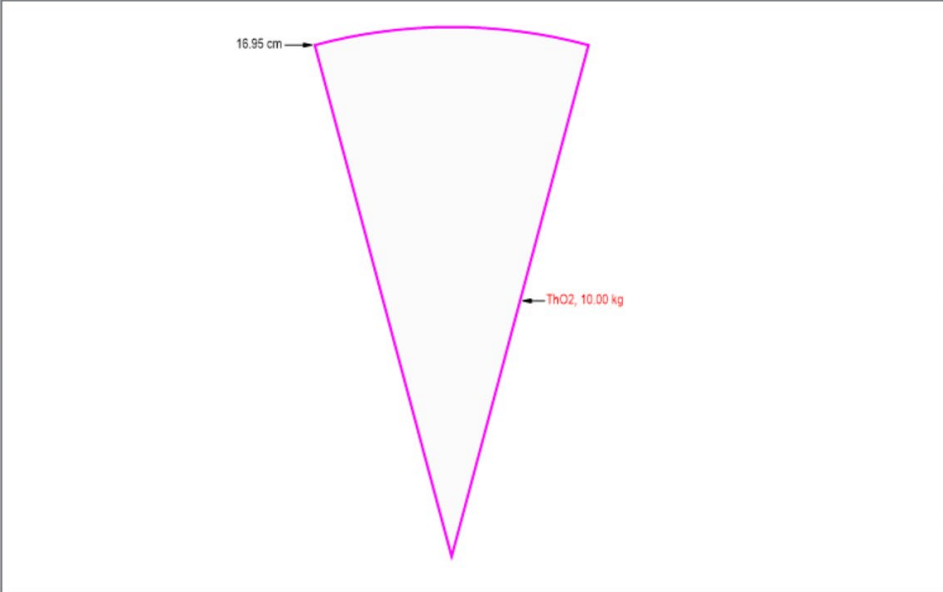
Appendix E: GADRAS Model Files

GADRAS 18.8.7 (64 bit) Handheld\Detective-EX100 (Neutron: Detective-EX100)

Detector Plot Time History Analyze **Model** Neutron Inject Tools Setup

File Edit View Shell Radiograph 3DM Help

Description: thorium ball
Model: ThoriumBall.1dm Shell: 1 Thorium Oxide (ThO2) Change



16.95 cm

ThO2, 10.00 kg

Model Specifications

Shell Specifications

Density (g/cc)	0.49	
Age (years)	20	
AD (g/cm2)	8.307	Sigma (%)
Thickness (cm)	16.952683	
Outer Rad. (cm)	16.952683	
Mass (kg)	10.0	

☐ Variable Width

Shell Extents

Shell Material

☒ Include Material Source Terms

Material	Trace Sources	
Nuclide	Amount (w/o)	Vary
O	12.1 %	<input checked="" type="checkbox"/>
Th232	87.9 %	<input type="checkbox"/>

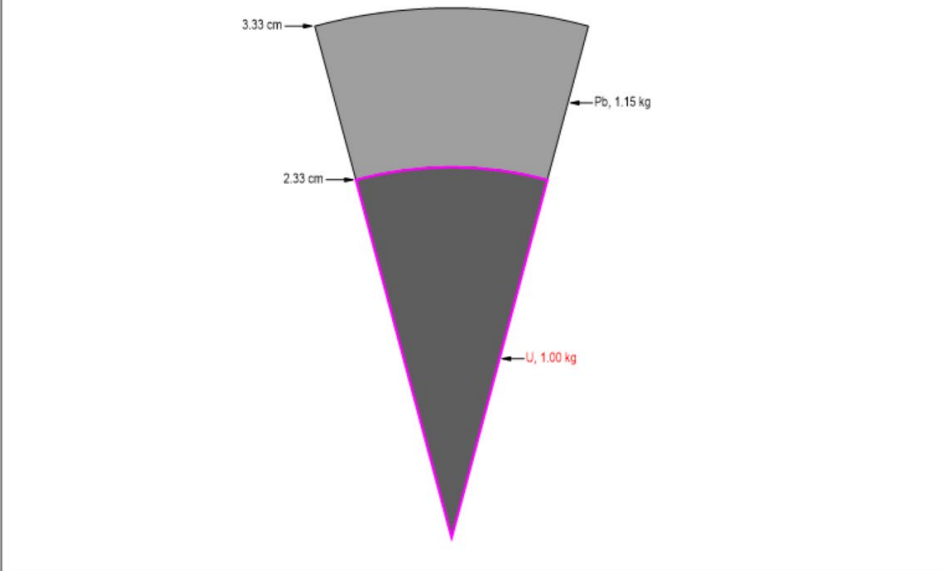
Save Material Normalize

GADRAS 18.8.7 (64 bit) Handheld\Detective-EX100 (Neutron: Detective-EX100)

Detector Plot Time History Analyze **Model** Neutron Inject Tools Setup

File Edit View Shell **Radiograph** 3DM Help

Description: U233 model
Model: U233ball.1dm Shell: 1 Uranium Metal (U) Change



3.33 cm

Pb, 1.15 kg

2.33 cm

U, 1.00 kg

Model Specifications

Shell Specifications

Density (g/cc)	18.95	
Age (years)	1	
AD (g/cm2)	44.094	Sigma (%)
Thickness (cm)	2.326845	
Outer Rad. (cm)	2.326845	
Mass (kg)	1.00	

☐ Variable Width

Shell Extents

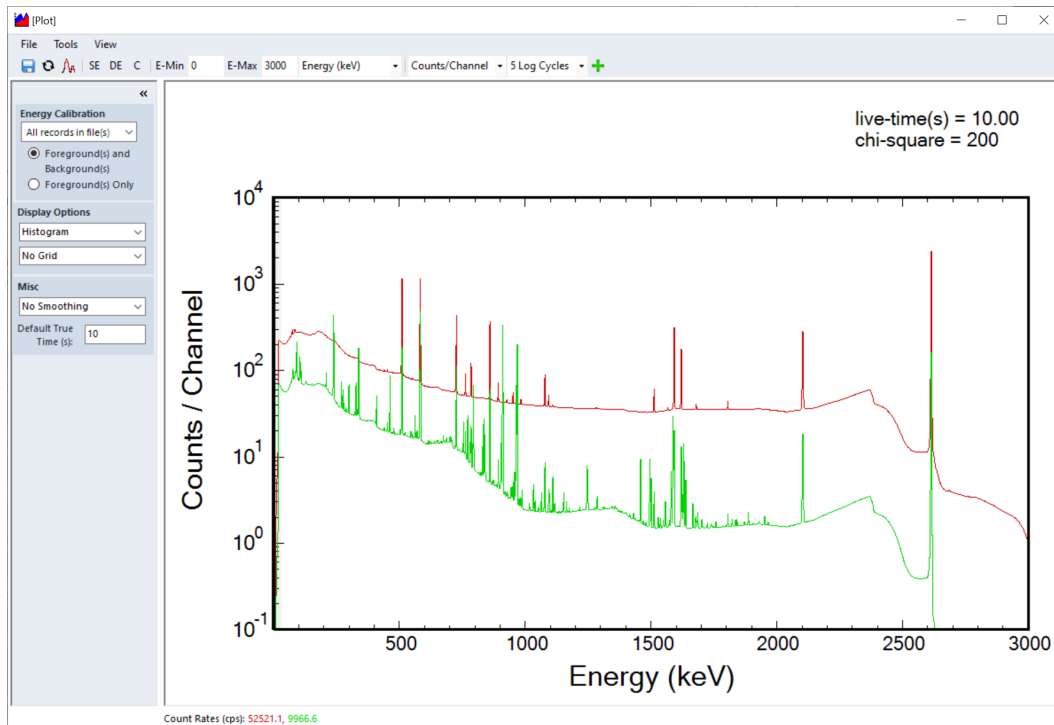
Shell Material

☒ Include Material Source Terms

Material	Trace Sources	
Nuclide	Amount (w/o)	Vary
U232	1.00E-03 %	<input checked="" type="checkbox"/>
U233	99.999 %	<input type="checkbox"/>

Save Material Normalize

Appendix F: Gam file physics information. (U233=red, Thorium=green). For ease of viewing the information is plotted after folding with a Detective EX-100 function. File header and tail text are also shown below.



```
GamFileVersion = 2.1
DataType = SnTransport 18.8.10.0
Geometry = Spherical
Description = thorium ball
LargestDimension = 3.391E+01
Data =
    568          92          79 ! photon lines, photon groups,
neutron groups
...
0.00298824091441929 ! k-eff
1.00299719726191 ! multiplication
```

```
GamFileVersion = 2.1
DataType = SnTransport 18.8.10.0
Geometry = Spherical
Description = U233 model
LargestDimension = 6.654E+00
Data =
    334          144          79 ! photon lines, photon groups,
neutron groups
...
0.465361446142197 ! k-eff
1.87042253646745 ! multiplication
```